4-Methylbenzenesulfonic acid
104-15-4 | DTXSID0026701

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.15

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 6.01e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
p-(Methylsulphonyl)benzoic acid	[3-(Methanesulfonyl)phenyl]acetic acid	4-Methylumbelliferone
Measured: 0.67	**Measured:** 0.06	**Measured:** 1.90
Predicted: 5.52e-01	**Predicted:** 5.04e-01	**Predicted:** 1.21